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1 Oct. 91 through 30 Sept 92

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Contract/Grant Number N00014-90-J-1370
Contract/Grant Title: SURFACE AND DEFECT EXCITATIONS
IN COVALENTLY BONDED SOLIDS

Principal Investigator: J.D. Joannopoulos

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- a. Number of Papers Submitted to Refereed Journals but not yet published: **None**
- b. Number of Papers Published in Refereed Journals: **11** (List Attached)
- c. Number of Books or Chapters Submitted but not yet Published: **None**
- d. Number of Books or Chapters published: **None**
- e. Number of Printed Technical Reports & Non-Refereed Papers: **None**
- f. Number of Patents filed: **1**
- g. Number of Patents Granted: **None**
- h. Number of Invited Presentations at Workshops or Prof. Society Meetings: **9** (List Attached)
- i. Number of Presentations at Workshops or Prof. Society Meetings: **None**
- j. Honors/Awards/Prizes for Contracts/Grant Employees: **3** (List Attached)
- k. Total Number of Graduate Students and Post-Docs Supported at least 25% this year on this contract grant:

Grad Students **1** and Post Docs **1**
Grad Student Female **0**
Grad Student Minority **0**
Grad Stud. Asian e/n **1**
Post-Doc Female **0**
Post-Doc Minority **0**
Post-Doc Asian e/n **0**

(b) Publications in Refereed Journals

1. A. Rappe, J.D. Joannopoulos and P. Bash, "A Test of the Utility of Planewaves for the Study of Molecules from First Principles", J. Am. Chem. Soc. **114**, 6466 (1992).
2. T. Arias, M. Payne and J.D. Joannopoulos, "Ab-Initio Molecular Dynamics at Large Length-Scales," Physical Review **B45**, 1538 (1992).
3. K. Cho and J.D. Joannopoulos, "Ergodicity and Dynamical Properties of Constant Temperature Molecular Dynamics", Physical Review **A45**, 7089 (1992).
4. K. Brommer, M. Needels, B. Larson and J.D. Joannopoulos, "Ab-Initio Theory of the S:(III) (7x7) Surface Reconstruction - A Challenge for Massively Parallel Computation", Phys. Rev. Lett. **68**, 1355 (1992).
5. E. Yablonovitch, T. Gmitter, K. Leung, R. Meade, A. Rappe, K. Brommer and J.D. Joannopoulos, "Electromagnetic Microresonators in 3D Photonic Band Structure", Optical and Quant. Elect. **24**, 273 (1992).
6. R. Meade, K. Brommer, A. Rappe and J.D. Joannopoulos, "The Existence of a Photonic Bandgap in Two Dimensions", App. Phys. Lett. **61**, 495 (1992).
7. R. H. Wolfe, M. Needels, T. Arias and J.D. Joannopoulos, "New Revelations in the Electronic Structure of Silicon as Derived from Volume Visualization of Ab-Initio Calculations", IEEE Computer Graphics and Applications, Vol 12, #4 (1992).
8. W.M. Robertson, G. Arjavalingam, R.D. Meade, A. Rappe, K. Brommer and J.D. Joannopoulos, "Measurement of Photonic Bandstructure in a Two-Dimensional Periodic Dielectric Array", Phys. Rev. Lett. **68**, 2023 (1992).

9. A. Rappe, A. Dal Pino, M. Needels and J.D. Joannopoulos, "Mixed Basis Pseudopotential Method for Iterative Diagonalization Techniques", Phys. Rev. B **46**, 7353 (1992).
10. T. Arias, M. Payne and J.D. Joannopoulos, "Ab-Initio Molecular Dynamics: Analytically Continued Energy Functionals and Insights into Iterative Solutions", Phys. Rev. Lett. **69**, 1077 (1992).
11. A. Dal Pino Jr., M. Needels, J.D. Joannopoulos, "Oxygen Induced Broken Bond Defect in Si", Phys. Rev. B **45**, 3304 (1992).

(h) Invited Papers

1. J.D. Joannopoulos (M. Needels, Y. Bar-Yam, S. Pantelides), APS Meeting March (1992).
2. A. Rappe (R. Meade, K. Brommer, J.D. Joannopoulos) , APS Meeting March (1992).
3. W. Robertson (G. Arjavalingam, R. Meade, K. Brommer, A. Rappe and J.D. Joannopoulos), Quant. Elect. and Laser Science Conf., Anaheim (1992).
4. K. Brommer (M. Needels, B. Larson and J.D. Joannopoulos), Electronic Structure Algorithms Workshop, North Carolina (1992).
5. J.D. Joannopoulos, Workshops and Grand Challenges in Structural Biology, Tallahassee, Florida (1992).
6. R. Meade (K. Brommer, A. Rappe and J.D. Joannopoulos), Electronic Structure Algorithms Workshop, North Carolina (1992).
7. K. Brommer (B. Larson, M. Needels and J.D. Joannopoulos), International Workshop on Nanometer Scale Sciences, Sendai, Japan (1992).

8. R. Meade (K. Brommer, A. Rappe and J.D. Joannopoulos),
New England Region AAPT Meeting, New London, CT (1992).
9. T. Arias, (J.D. Joannopoulos), Eur. Res. Conf. on El
Structure of Solids, Cambridge (1992).

(j) Honors, etc.

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|-----------------|-----------------------------|
| 1. Andrew Rappe | JSEP Fellowship |
| 2. Tomas Arias | AT&T Bell Labs Fellowship |
| 3 Kyeongjae Cho | Korean Overseas Scholarship |

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